Report from the Subcommittee on the Evaluation of the Long Term Goal of Enabling Effective Modeling of Complex Systems.

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Charge: The subcommittee was asked to evaluate progress toward the long term goal:
"By 2015, demonstrate progress toward developing the mathematics, algorithms and software that enable effective scientifically critical models of complex systems, including highly nonlinear or uncertain phenomena, or processes that interact on vastly different scales or contain both discrete and continuous elements."

Evaluation: The subcommittee finds that OASCR has made an excellent start toward achieving the goal of enabling effective modeling of complex systems, in particular those systems with processes that interact on vastly different scales.

ASCR has so far initiated two efforts to address the long term goal of enabling effective modeling of complex systems. To get started, OASCR rightfully focused on advancing multiscale mathematics to address processes that interact on vastly different scales as there is widespread agreement that multiscale mathematics is an area ripe for the greatest payoffs. This first effort has progressed and matured to a funded program, which is where this subcommittee has focused its evaluation. The Multiscale Mathematics Research and Education Program was initiated in 2004 with a series of workshops to define the opportunity and a path forward. A second effort that will begin a process similar to the multiscale effort, but to address a broader set of mathematical challenges in the field of Complex Systems, will begin with a workshop scheduled for December 7-8, 2006. Because of the infancy of the second effort, the subcommittee chose to only briefly comment herein that the planned workshop addresses an important set of challenges underlying essential phenomena for which neither current mathematical methods nor multiscale mathematics adequately address. This subcommittee finds, nevertheless, that the complex systems workshop is well along in its planning, and the effort shows enormous promise. This finding is based on the credentials and dedication of the organizers and the invitation list developed by those organizers.

The Multiscale Mathematics Program was launched with a series of three workshops in May, July, and September of 2004. The participants in these workshops were broadly representative of the mathematics and computational science community. Three excellent reports were produced, the third of which attempts to summarize all three workshops. The result of these workshops was a strategic plan for addressing the mathematical challenge of multiscale phenomena and has yielded the desired outcome of increasing awareness of the program and its research challenges in the mathematics and computational science community. (The RFP and workshop reports can be accessed at: http://www.sc.doe.gov/ascr/mics/ams/index.html)

One important conclusion from the workshops is that modeling multiscale phenomena is an endeavor that will not be advanced by solely increasing computer hardware capability.

Addressing problems with widely disparate scales using existing algorithmic techniques would require computing capability that, assuming Moore's law of increasing computer speed, will not be available this century. Enabling effective modeling of complex systems involving interacting processes on a vast range of scales by 2015 will necessarily require the development of new mathematics and new algorithms and will also require collaborations amongst domain scientists who have developed the modeling applications, as well as understand the phenomena, with mathematicians and computer scientists who can develop new mathematical and computational approaches.

The request for proposals was posted January 7, 2005, closed March 28, 2005, and awards were announced on August 4, 2005. Of the 170 proposals received, only 13 were funded. Those 13 awards involve 25 institutions, 17 of which are universities and 8 are DOE laboratories. The total amount of funding awarded is ~$20.6M for three years. The first opportunity to initiate new projects might be in FY08. (A spread sheet with the award titles, institutions, and PIs as well as the original press release with funding levels is attached.)

This subcommittee was not provided access to the proposals, nor to any specific information on the selection process, other than to find that OASCR convened two expert panels, one to evaluate proposals submitted with a DOE laboratory as the lead and the other for proposals submitted with an academic institution as the lead.

The subcommittee read all the first year progress reports albeit with limited context. The subcommittee notes that the awards range from single PI proposals to projects involving large teams from several universities and laboratories and funding levels ranging from a minimum of $650K to a maximum of $2.6M for three years. The Average three year award was ~$1.6M. The applications addressed in these projects cover a good cross-section of important problems, ranging from biological systems to plasma physics, from nanoscale materials to climate modeling. It is clear that if these projects are successful, good progress towards the long term goal will have been achieved.

The subcommittee observes that, while a number of the projects have assembled interdisciplinary teams that include mathematicians, numerical analysts, and computer scientists along with application scientists, there are also a number of projects that lack similar breadth. As stated above, the achievement of the goal of enabling effective modeling of multiscale complex systems will require new mathematics that is not application specific and new algorithms focused on classes of problems. The subcommittee holds the view that the most promising approach would be to include expertise across the entire spectrum within each proposal. Future award strategy should keep this in mind.

The subcommittee also observes that, without additional funding, the first opportunity to initiate new projects will be in FY08. We urge OASCR to seek additional funding for this critically important portfolio. The fact that 170 proposals were reviewed, and probably 80% had significant promise, but only 13 awards were made suggests that many excellent projects went unfunded. However, it is imperative that additional funding not come from

the core applied and computational mathematics budget, which needs to maintain its portfolio breadth. We again emphasize that this program, and the program to be formulated in the pending Complex Systems Workshop, will not achieve their goals without new mathematics and new algorithmic development. To constrain the growth of these programs as a lower priority to additional investments in computer hardware would make achieving the goal difficult at best.

ATTACHMENTS

List of Projects	Press Release
Multiscale Mathematics Researc	Multiscale Math Press Release

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